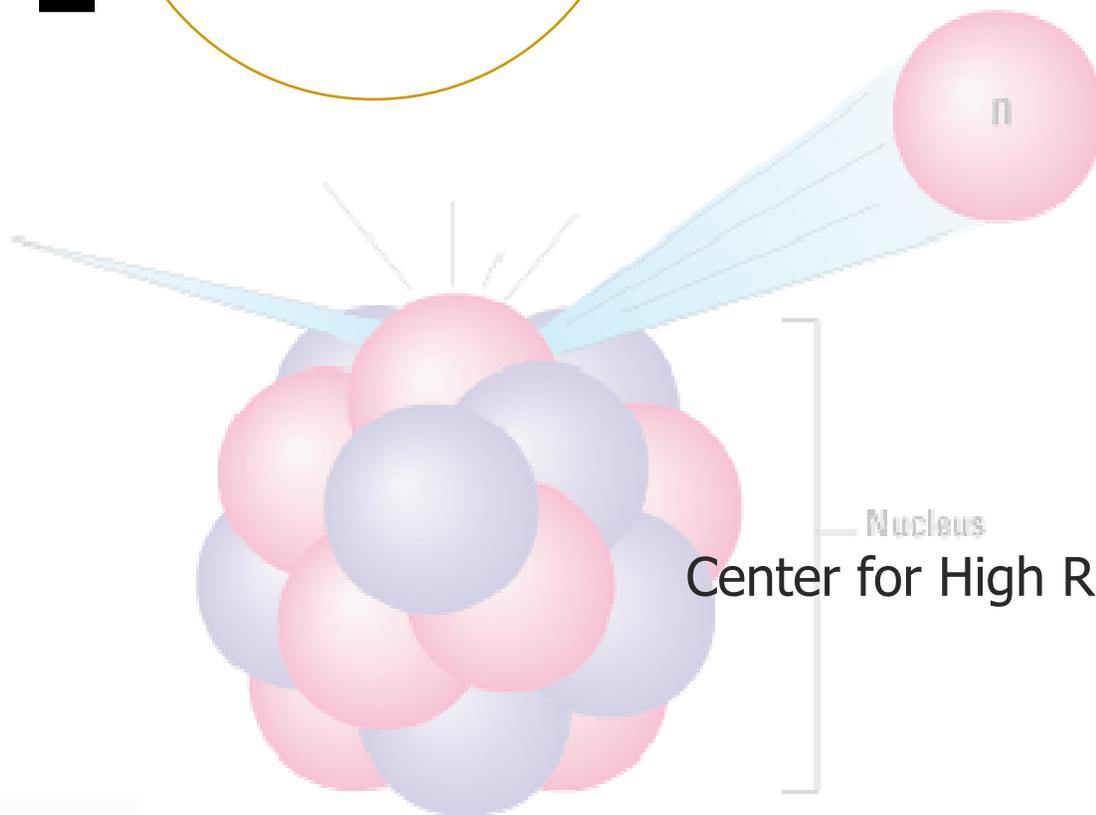


*and FANS*

# High Flux BackScattering

Quantum rotations in Methyl Iodide<sup>^</sup>



Group D

June 27<sup>th</sup>, 2007

Summer School 2007

Center for High Resolution Neutron Scattering

NIST

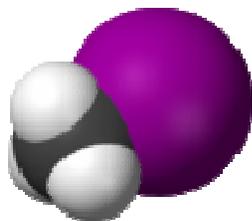
- Caleb Dyer
- Cary Pint
- Jacob Tarver
- Kokonad Sinha
- Margaret Johnson
- Mark Snyder
- Sheila Khodadadi
- Yang Zhang



# Methyl Iodide

## Bulk dynamics

NIST



**Bulk CH<sub>3</sub>I dynamics:**  
Simplified model based on symmetry alone:

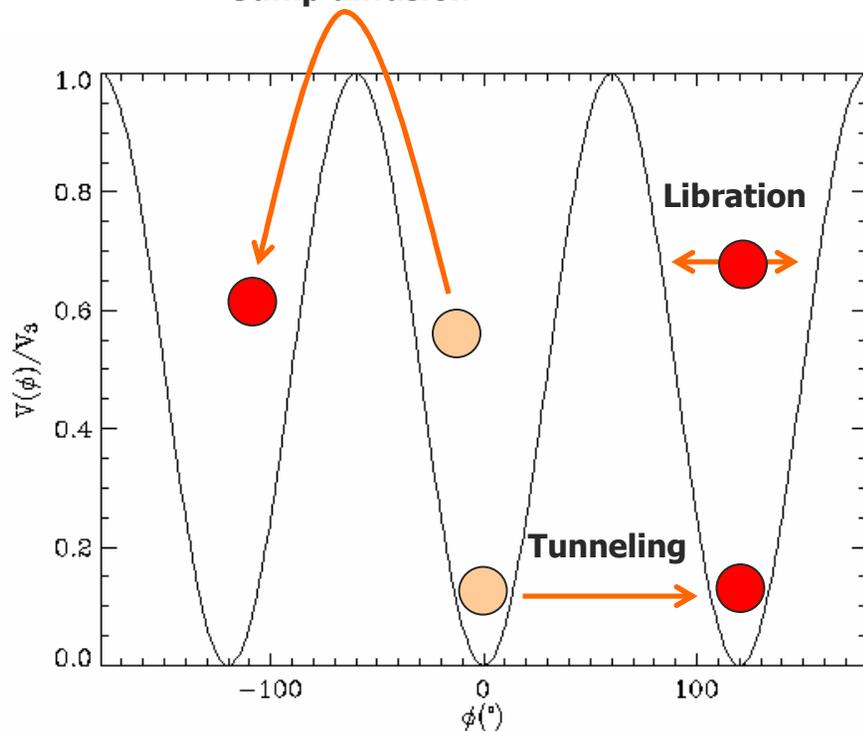
$$V(\phi) = V_3 \frac{(1 - \cos(3\phi))}{2}$$

Solution of Hamiltonian from

$$H = -B \frac{d^2}{d\theta^2} + \frac{V_3}{2} (1 - \cos 3\theta)$$

Tunneling rate proportional to overlap of wave functions through the barrier  
Overlap increases with librational level.

**Jump diffusion**



**Why methyl iodide?**

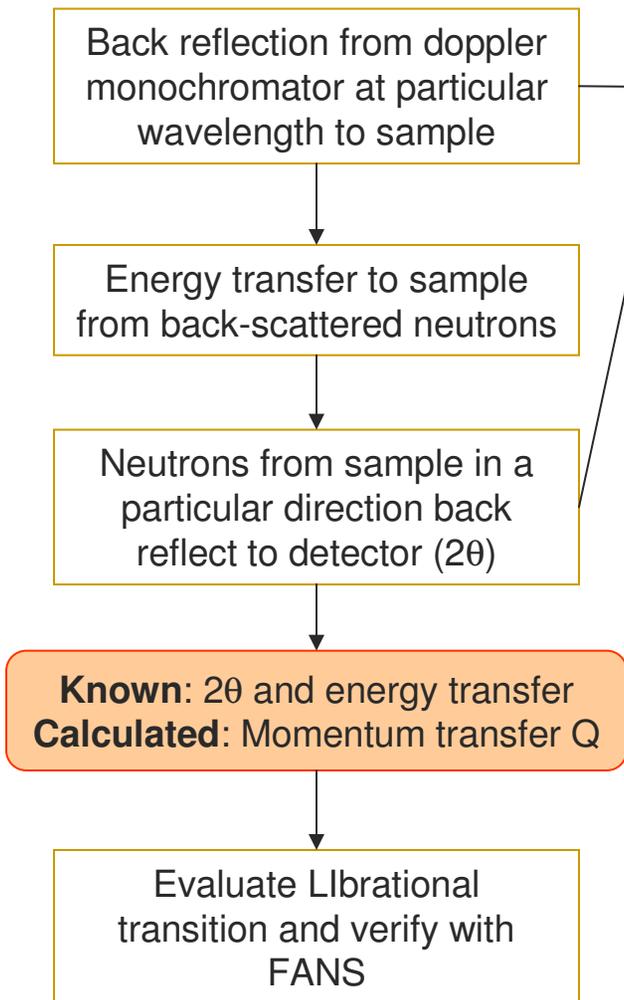
Many scattering events in a short amount of time

**Objective:**

- Through tunneling experiment, predict:
- Potential barrier height
  - Radius of methyl group
  - Librational transition
  - Verification by FANS

# Methodology

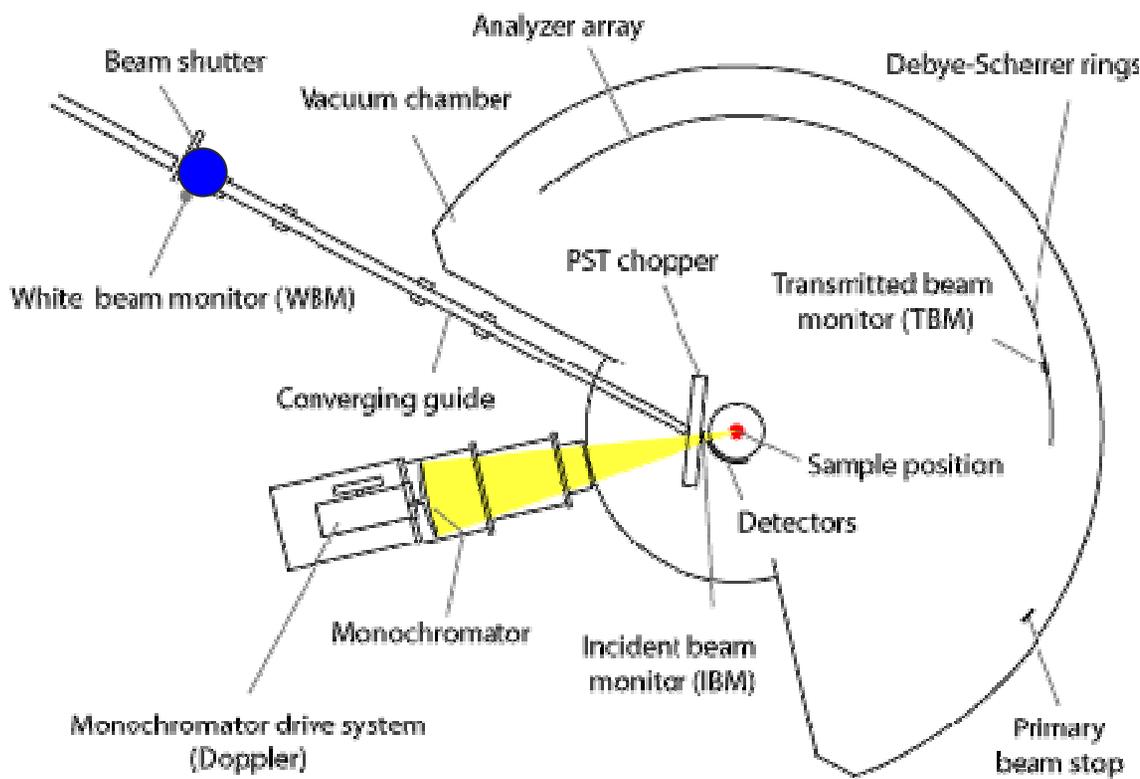
## Using the HFBS instrument



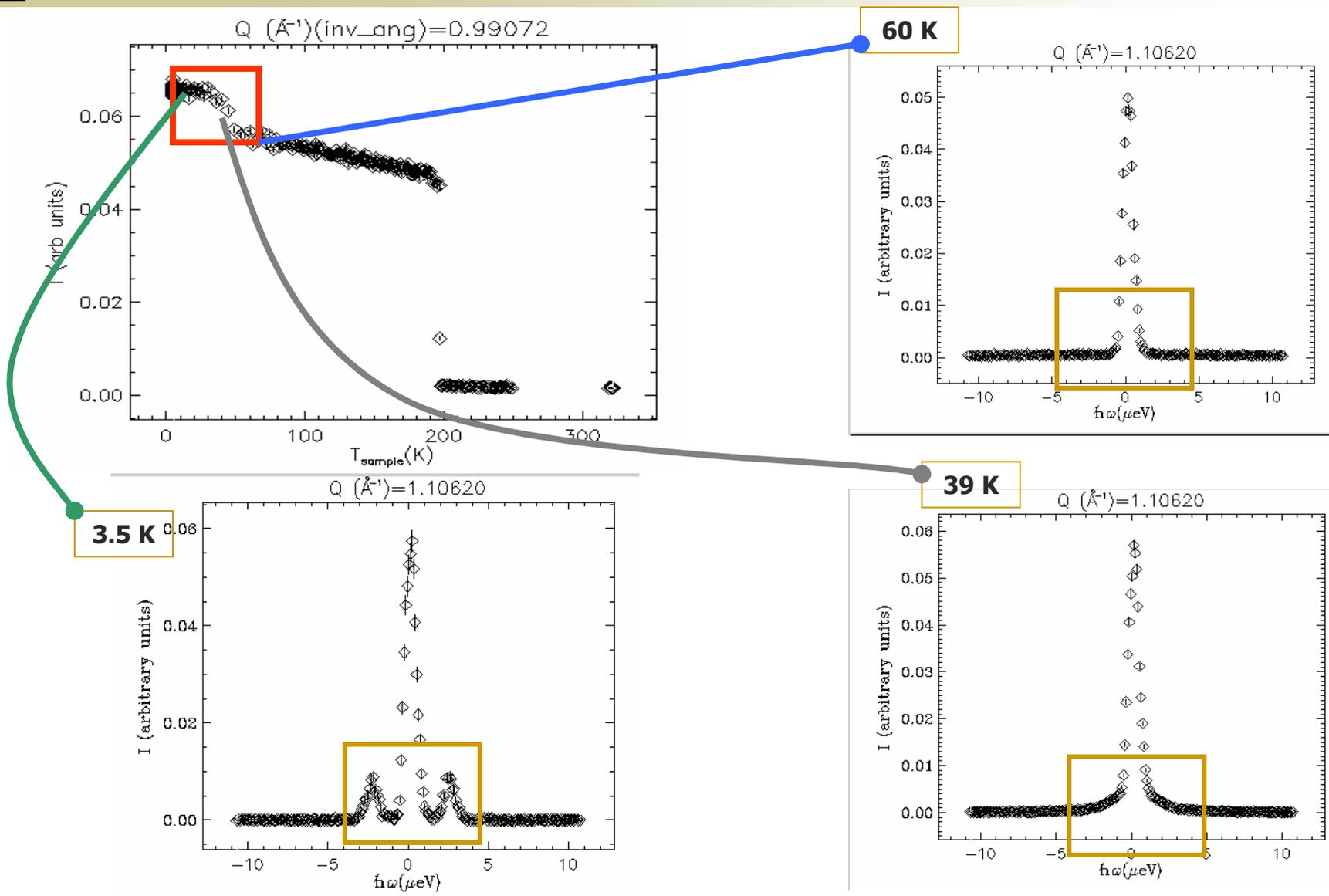
Energy window:  
-11 to +11 meV

Energy: 2.08 meV

- Issues to deal with**
- Thickness of sample
  - Multiple scattering
  - Sample geometry
  - Energy-dependent background



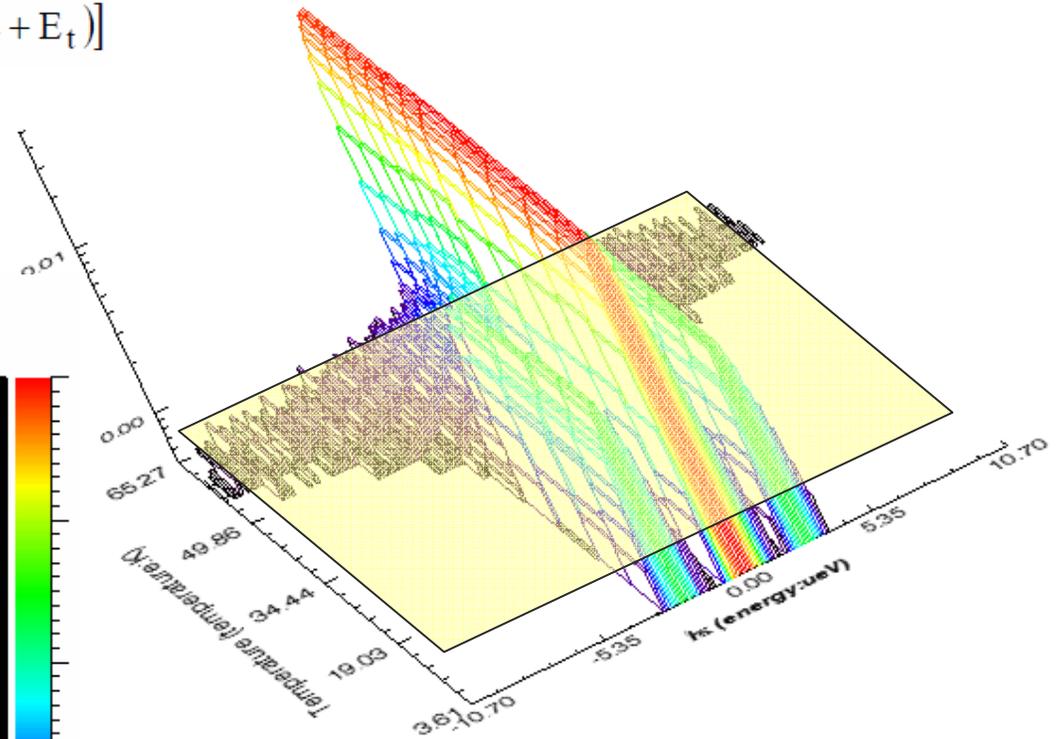
# Choosing temperatures



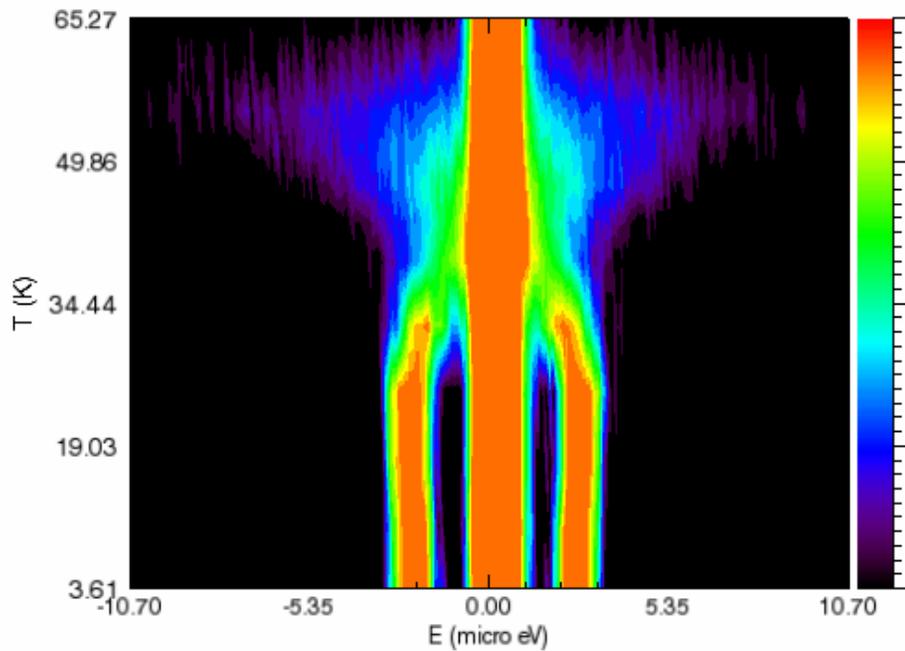
$$S(Q,E) = A_0(Q)\delta(E) + \frac{(1-A_0(Q))}{2} [\delta(E - E_t) + \delta(E + E_t)]$$

Elastic

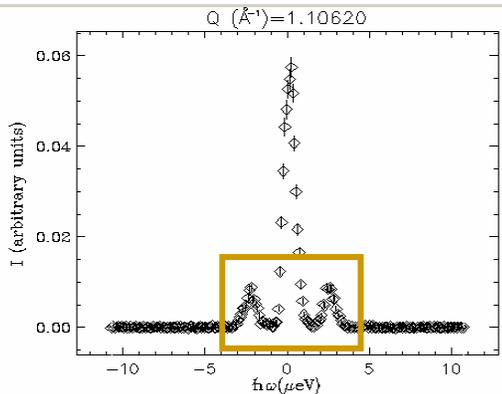
Inelastic



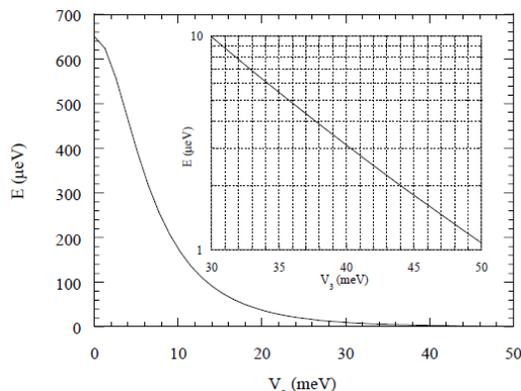
Intensity Contour



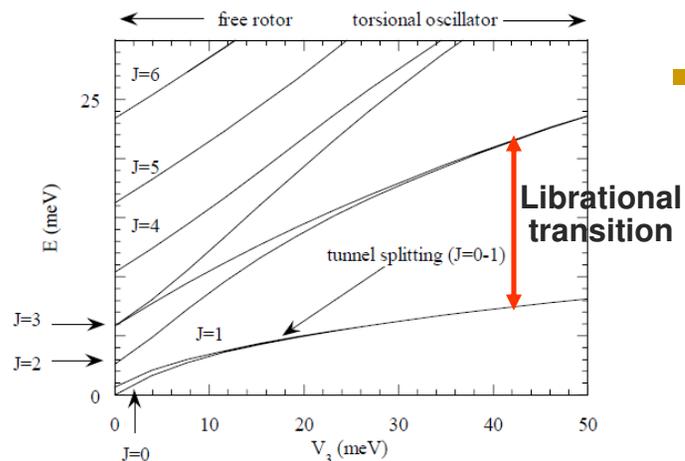
# Calculations



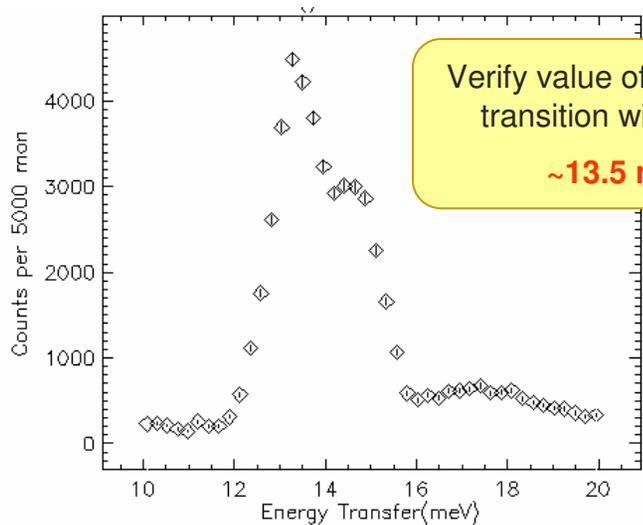
Obtain location (energy) of inelastic peak



Obtain potential  $V_3$  from graph of transition energy vs. potential ( $\sim 42$  meV)



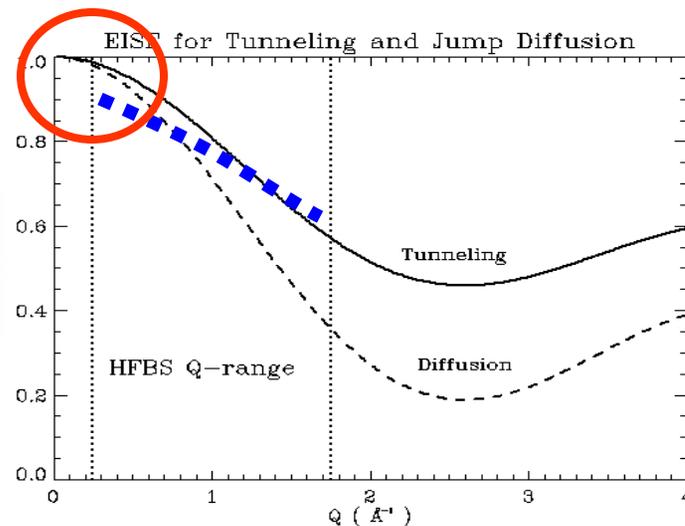
Obtain Librational transition!  
**15.6 meV**



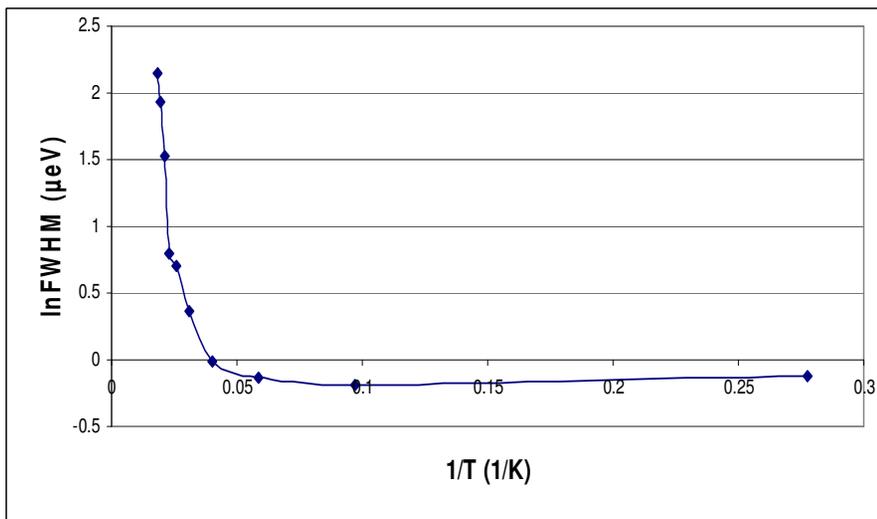
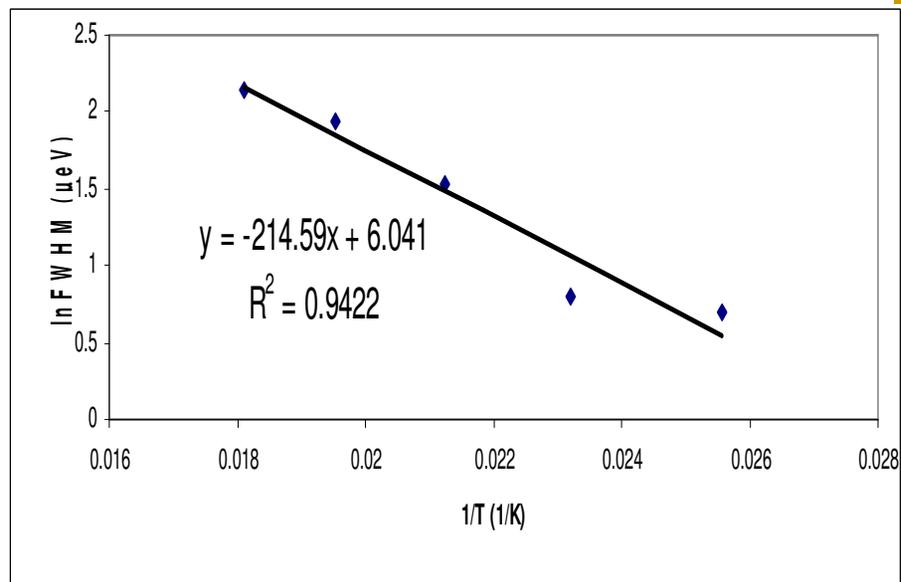
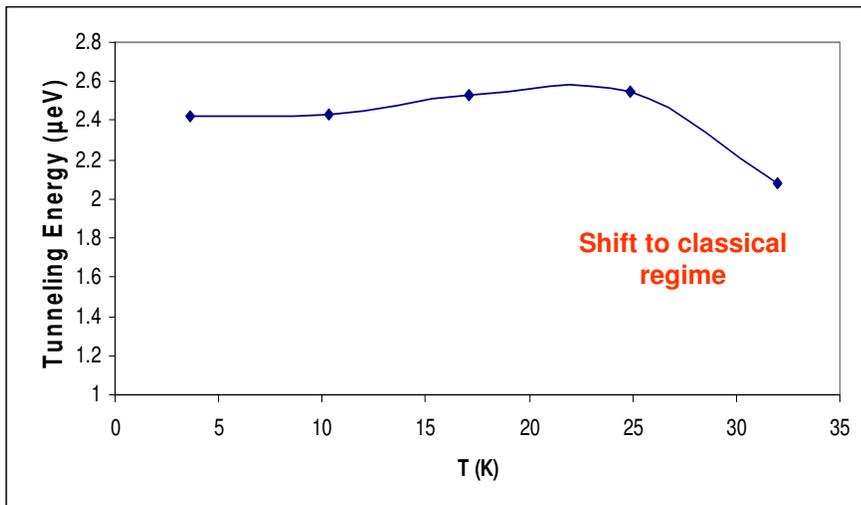
Verify value of Librational transition with FANS  
 **$\sim 13.5$  meV**

$$A_0(Q) = \frac{5 + 4j_0(Qr\sqrt{3})}{9}$$

**$R \sim 0.97 \text{ \AA}$**



# More observations



Obtained activation energy = 18 meV

- The HFBS team
  - Victoria Garcia Sakai, Juscelino Leao and Robert Dimeo
- FANS: Terrence Udovic
- Antonio Faraone, Yamali Hernandez, Julie Keyser
- All instrument specialists!
- NCNR at NIST

Thank You  
*Grazie* Takk

DANKE  
*Merci*  
Thanks  
*Gracias*  
Thank You  
*Obrigado*